

Evidence for an *I2/a* to *Imab* phase transition in the silica polymorph moganite at ~570 K

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ABSTRACT

Rietveld analysis of synchrotron X-ray powder diffraction data for the silica mineral moganite from 100 K to 1354 K has revealed a reversible phase transition from space group *I2/a* to *Imab* at approximately 570 K. The thermal expansion behavior of the lattice parameters alters sharply at the transition point, and the monoclinic β angle decreases to 90°. The displacive transition from α - to β -moganite is effected by the rotation of apparently rigid tetrahedra about the [010] axis, and the linear temperature dependence of the volume strain and of the non-symmetry-breaking e_{11} and e_{22} strains indicates that the character of the transition is second-order. The continuous increase in the **b** axis over the entire temperature range reveals a concomitant rotation of tetrahedra about [100] that does not affect the overall symmetry. In addition, we present a refinement without structural constraints for α -moganite at room temperature using time-of-flight neutron diffraction data.